

Reagan proposes increasing federal
R&D funding 16% next year
Page 9

FEBRUARY 17, 1986

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Slow but solid growth
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CHEMICAL & ENGINEERING NEWS

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News of the Week

■ **EPA must have a broader program on biotechnology, expand research on health effects, Biotechnology Study Group says.** Page 6

■ **Efforts of human rights activists, U.S. and European scientists rewarded by release of computer scientist Anatoly Scharansky from the Soviet Union.** Page 7

■ **Du Pont will spend only \$1.12 billion on R&D this year, 4% below the 1985 level.** Page 7

■ **Chemical industry executives and Senators from northeastern states oppose tax on imported oil proposed as method of reducing federal budget deficit.** Page 8

■ **Ban on chemical weapons nudges closer to reality as U.S. and Soviet actions indicate shifts in approach to meet that goal.** Page 8

News Focus

R&D funding increases 17% over 1986 figures in Administration's proposed 1987 budget; DOD gets almost 70% of the total. Page 9

Business

Natural gas-based chemicals ammonia, urea, and methanol losing markets to countries with lower-cost feedstocks. Page 16

Agriculture slump causes shortage of water fluoridation chemicals, by-products of phosphoric acid production. Page 20

Government

Department of Defense funding of university research has increased substantially since 1980 and SDI will accelerate it. Page 23

Science

Uranus as pictured by Voyager 2 has a uniquely oriented magnetic field, nine dark rings, geologically different moons. Page 53

Applying data on beryllium, x-ray crystallographers derive quantum mechanically meaningful wave functions for atoms. Page 58

Books

"Going Sour: Science and Politics of Acid Rain" by Ray Gould is a less than even-handed treatment of the issue. Page 59

Cover: Harshaw Filtril employee displays nickel catalysts

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Product Report

Process catalysts, used in petroleum refining and in chemical processes, are a steadily growing business in the U.S. Page 27

Funds for R&D Are Up 17% in Administration's Budget Proposal

Department of Defense R&D budget consumes large percentage, just under 70%, of total R&D budget; proposed funding for overall basic research is up 8%, whereas that for applied research is down 2%

Janice R. Long, David J. Hanson,
and Wil Lepkowski, C&EN Washington

According to acting Presidential Science Adviser John P. McTague, the proposed 1987 budget that the Administration sent to Capitol Hill on Feb. 5 "reflects three guiding priorities: to stop signing our children's names to IOUs for our own pocket money; to ensure a stable, secure nation and world by continuing to modernize our defensive forces; and to provide the scientific, technical, and human resource base to maintain the nation's leadership in an increasingly competitive marketplace."

The two last priorities are accurately reflected in the proposed 1987 federal R&D budget, as is the Administration's commitment to basic research as opposed to applied research and development work. In an overall federal budget that is up only 1% from 1986

to \$994 billion, R&D obligations are up 17%, or \$8.8 billion, to \$60.8 billion, and outlays are up 7%, or \$3.6 billion, to \$51.4 billion.

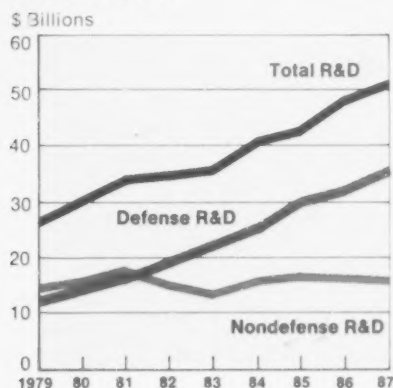
Those figures do not include funds for R&D facilities, which, if factored in, result in a 1987 increase in R&D obligations of 16% over 1986 funding levels to \$62.5 billion. Overall obligations for R&D facilities are down 4% to \$1.7 billion, and outlays are up 2% to the same figure.

Obligations for basic research are going in the opposite direction, up 8%, or \$615 million, to \$8.6 billion. Outlays for basic research are up 5%, or \$364 million to \$8.3 billion. Obligations for applied research are down 2%, or \$141 million, to \$5.5 billion, and obligations for development are down 10%, or \$347 million, to \$3.2 billion.

Since the Reagan Administration took office in 1981, funding for federally sponsored development work

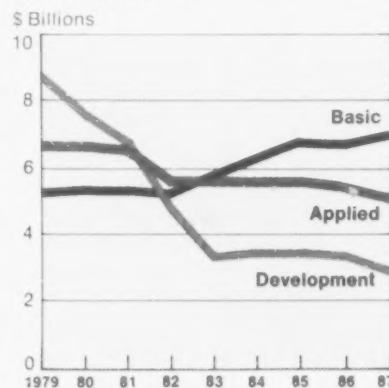
Under the Reagan Administration,

spending for defense R&D
has risen 50% . . .



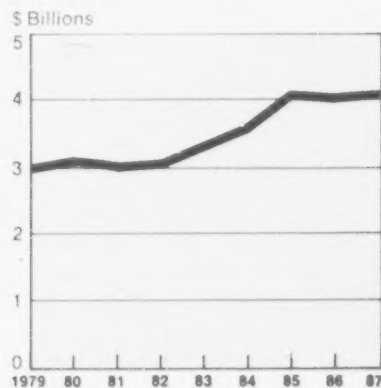
Note: Outlays. Source: Office of Management & Budget

. . . for nondefense basic research
more than 30% . . .



Note: Obligations in constant 1985 dollars. Source: Office of Science & Technology Policy

. . . and for academic research
about 35%



has dropped some 44%, and funding for applied research has dropped 8% in terms of constant 1985 dollars. Funding for basic research, on the other hand, has risen 30%, with the share going to colleges and universities rising 18% to some \$6.4 billion in fiscal 1987.

The Department of Defense budget for research, development, testing, and engineering is consuming an ever larger percentage of the federal R&D budget. In 1986 it accounts for just under 65% of total R&D obligations, in 1987 just under 70%, according to Office of Management & Budget calculations. (R&D numbers obtained from individual agencies frequently differ from those used by OMB in preparing its analyses, known as Special Analysis, of total federal R&D funding.)

DOD's proposed RDT&E budget for 1987 is \$41.9 billion, for an increase of \$6.4 billion, or 18%, above the level funded in 1986. Most of that money does not support what is traditionally called research and development, but rather the testing of advanced tactical weapons systems and other engineering tasks. The portion of the budget that funds basic research, referred to as the technology base, is comparatively small. At slightly less than \$3.6 billion, it represents less than 9% of the total RDT&E budget.

Quite a bit of that research money would be devoted to the Strategic Defense Initiative, the so-called Star Wars program, for defense against nuclear attack. Overall funding for SDI is proposed to increase to \$4.8 billion for 1987, up from \$2.75 billion obligated for 1986. (For the impact this growing source of funds has on universities, see story on page 23.) The SDI program began in 1985 with about \$1.5 billion and so has grown about 300% in three years.

In other programs, the military services plan to double their spending at universities for graduate scholarships and assistantships, proposing about \$50 million for 1987. This initiative was started just last

year, and DOD proposes another doubling of funds for it in fiscal 1988. Total research support from DOD to universities will top \$1 billion for the first time in 1987, and more than half of that will go to basic research. However, with the emphasis on technology development, it is estimated that only about \$85 million will be for basic research in chemistry.

Among the big money items touted by Defense officials at the opening rounds of budget hearings is development of the JVT tilt-rotor aircraft, which is designed for rapid troop transport, and development of a new, faster, quieter attack submarine with an advanced combat system. Work on the MX, or Peacekeeper, missile continues with development support for the second 50 of these multiple-warhead missiles. Chemical weapons continue to be pushed by the Joint Chiefs of Staff, and new funds are requested for work on these.

In contrast to the skyrocketing defense RDT&E funding, the Administration once again is proposing a decrease in R&D support for the Department of Health & Human Services, down 1% to \$5.47 billion. Virtually all the loss would come from the National Institutes of Health, which is scheduled to receive a cut of \$478 million, or 9%, to \$4.9 billion.

The Administration has made a careful study of what it wants from NIH, particularly after the battle it lost with Congress last year over the appropriate number of new and competing research grants. Congress passed a budget to fund 6500 such grants each year that was vetoed by the President. Congress compromised and overrode the veto, allowing NIH to increase its funding from about 5000 to 6000 new grants yearly.

HHS proposes in the 1987 budget that NIH fund 18,000 total grants, not just new grants, each year from a total of \$2.8 billion. The average award would be \$156,700, an increase of 2% over 1986. At present total grants may number about 18,300. HHS says that the new method of funding would provide more stability to the grants process and that NIH will be able to be more cost conscious in the review and approval of grants. To provide for a smooth transition to the 18,000-grant total, the Administration has sent a number of rescission proposals to Congress asking that some \$23 million be deleted from NIH's fiscal 1986 budget.

One area where HHS hopes to find some savings is indirect costs. The Administration is proposing a 20% limit on administrative overhead for research projects, a move expected to save \$86 million in 1987. The current average indirect cost levied on grants is 26%, according to the HHS Office of the Inspector General.

In other areas of HHS-sponsored R&D, the Food & Drug Administration would get an increase of \$40 million to \$424 million in fiscal 1987. Likewise, the proposed budget for the Centers for Disease Control is up \$13 million to \$380 million next year. The Administration is also proposing a smaller increase, \$11 million, to go to the Alcohol, Drug Abuse & Mental Health Administration, raising its total to \$928 million.

The Department of Energy remains the third largest federal funder of R&D, resulting from a sharp rise in

Glossary of budget terms

Fiscal year. Year running from Oct. 1 to Sept. 30. The fiscal year is designated by the calendar year in which it ends.

Obligations. Commitments made by federal agencies to pay out money for products, services, or other purposes, as distinct from the actual payment.

Outlays. Payments for obligations incurred under Congressionally granted budget authority generally made by issuance of checks on the Treasury. Outlays during any fiscal year may be for obligations incurred in previous fiscal years or in the same fiscal year.

Rescission. Enacted legislation canceling budget authority previously granted by Congress. Rescissions proposed by the President must be approved by Congress within 45 days to become effective.

Federal R&D funding would rise 17% overall . . .

\$ Millions	Obligations			Outlays		
	1987 ^a	1986 ^a	1985 ^b	1987 ^a	1986 ^a	1985 ^b
Defense	\$41,823	\$33,485	\$31,099	\$32,693	\$29,267	\$27,878
HHS	5,471	5,524	5,444	5,532	5,561	4,997
Energy	4,886	4,785	4,901	4,819	4,778	4,900
NASA	4,051	3,594	3,235	3,743	3,528	2,970
NSF	1,508	1,334	1,346	1,455	1,338	1,186
Agriculture	907	922	941	911	913	889
Interior	345	381	389	351	403	414
EPA	310	334	320	332	318	275
Commerce	297	380	399	311	383	373
Transportation	277	364	430	331	416	417
Agency for International Development	203	206	210	209	208	204
Veterans Administration	194	186	227	187	182	215
All other	531	531	550	544	538	527
TOTAL	\$60,803	\$52,026	\$49,491	\$51,418	\$47,833	\$45,245

^a Estimate. ^b Actual. Note: Facilities funding not included.
Source: Office of Management & Budget

. . . with basic research funding up 8% . . .

\$ Millions	Obligations			Outlays		
	1987 ^a	1986 ^a	1985 ^b	1987 ^a	1986 ^a	1985 ^b
HHS	\$3353	\$3290	\$3229	\$3381	\$3303	\$2954
NSF	1423	1256	1262	1372	1260	1111
NASA	1085	857	728	1018	870	705
Energy	1045	922	926	1018	907	896
Defense	987	940	860	759	834	705
Agriculture	434	434	447	427	423	406
Interior	118	132	131	121	145	142
Smithsonian Institution	79	71	71	73	66	61
EPA	37	39	39	38	36	25
Commerce	20	22	23	20	21	23
Veterans Administration	16	15	15	15	15	16
Education	10	11	12	11	6	6
All other	25	28	27	27	30	26
TOTAL	\$8632	\$8017	\$7770	\$8280	\$7916	\$7075

^a Estimate. ^b Actual. Source: Office of Management & Budget

. . . and funds for facilities down 4%

\$ Millions	Obligations			Outlays		
	1987 ^a	1986 ^a	1985 ^b	1987 ^a	1986 ^a	1985 ^b
Energy	\$ 759	\$ 813	\$ 909	\$ 826	\$ 902	\$ 958
Defense	453	437	533	376	325	404
NASA	332	279	268	310	271	247
NSF	84	68	74	81	68	64
Agriculture	42	92	41	69	48	34
HHS	10	54	43	27	46	43
All other	54	68	27	41	30	34
TOTAL	\$1734	\$1811	\$1895	\$1730	\$1690	\$1784

^a Estimate. ^b Actual. Source: Office of Management & Budget

its defense-oriented research activities. Overall, DOE's R&D obligations would rise 3%, or \$155 million, to \$5.3 billion in fiscal 1987. Its defense R&D activities are slated to rise 19%, or \$429 million, to \$2.7 billion. That leaves civilian research programs with a 10%, \$275 million decrease to \$2.6 billion.

Despite the overall decline, there are some bright spots in DOE's civilian research program. Funding for supporting research and technical analysis would increase 6% to \$551 million. Within that total, operating expenses for the chemical sciences program, which were down slightly in fiscal 1986 because of the automatic Gramm-Rudman-Hollings deficit reduction law cuts, are up 11% to \$86.4 million. The program's capital equipment budget would rise 12% to \$9.6 million, whereas the construction budget would decrease 3% to \$5.4 million.

The operating budget for materials sciences research is slated to increase 17% to \$157 million. The capital equipment budget would rise 29% to \$15.5 million, but the construction budget would fall 44% to \$23.9 million. In other areas, university research support would rise 7% to \$11 million; however, funding for university research instrumentation would fall 21% to \$5 million.

Sliding very steeply is DOE's fossil energy R&D budget, down 56% to \$150 million. Within that program, funding for coal R&D, which includes a fair amount of chemical research, would fall even further—67% to \$82.2 million. Proposed funding for conservation R&D is down 54% to \$71.2 million, solar R&D down 47% to \$92 million, and nuclear energy programs are down 12% to \$333 million. Within the last category, however, funding for one program—space and defense power systems—would increase a dramatic 250% to \$71.7 million. The program focuses on developing nuclear power sources to support emerging DOD requirements for a variety of terrestrial and space missions, including SDI.

Exactly what will happen at the National Aeronautics & Space Administration is a mystery. Following the tragic loss of the space shuttle *Challenger*, the acting NASA administrator has vowed no more shuttles will be launched until their safety is assured. What that will do to shuttle expenses, now the greatest part of the NASA budget at about \$3.1 billion for its launches and communications controls, cannot be guessed. Acting NASA Administrator William R. Graham says the shuttle will continue to be the U.S.'s principal space transportation system.

R&D spending for NASA is slated at \$3 billion for 1987, a 9% increase that is somewhat better than the 3% overall increase NASA is requesting. The R&D funds will go toward initiation of space station development, with \$410 million spent to complete initial design work. Funds also will go to a new aerospace plane technology program. A major new program, one of the very few to be proposed in recent years, is Topex. Nearly \$30 million will support this ocean topography experiment, to be conducted jointly with France. To be launched in 1991, it will be a satellite system that gives oceanographers the first opportunity to observe currents on a global scale.

HOW THE AGENCIES FARE

Defense items boost DOE research budget

\$ Millions	1987 ^a	1988 ^a	1989 ^a	% change 1988-87
Weapons R&D, testing	\$2101.2	\$1729.8	\$1540.8	21%
Energy supply R&D	1599.5	1693.5	1818.8	-8
Supporting research and technical analysis	551.9	519.7	516.0	6
Magnetic fusion	333.0	365.4	429.5	-9
Nuclear energy	332.7	377.4	392.5	-12
Environment	273.8	228.6	230.5	20
Solar and other renewables	91.9	173.6	210.2	-47
Electric energy systems and storage	16.2	28.8	40.1	-44
General science and research	773.4	681.4	721.8	17
Naval reactors development	593.6	535.7	500.4	11
Fossil energy R&D	150.1	343.0	337.1	-56
Conservation R&D	71.2	170.9	151.6	-54
TOTAL	\$5289.0	\$5134.3	\$5170.5	3%

a Estimate. b Actual. Source: Department of Energy, S. Rept. 99-110

NSF's total budget is up 8% . . .

\$ Millions	1987 ^a	1988 ^a	1989 ^a	% change 1988-87
Mathematical and physical sciences	\$ 449.3	\$ 410.0	\$ 397.2	10%
Astronomical, atmospheric, earth, and ocean sciences	383.2	362.6	353.0	6
Biological, behavioral, and social sciences	282.4	260.1	253.5	9
Engineering	185.5	162.5	150.6	14
Antarctic program	117.0	115.2	110.8	2
Science and engineering education	89.0	87.0	82.0	2
Program development and management	78.0	72.5	72.0	8
Advanced scientific computing	53.6	45.2	41.4	19
Scientific, technological, and international affairs	47.0	39.5	43.7	19
Special foreign currency	0.7	1.0	2.8	-30
TOTAL	\$1685.7	\$1555.8	\$1507.0	8%

a Estimate. b Actual. Source: National Science Foundation

. . . as is funding for the sciences . . .

\$ Millions	1987 ^a	1988 ^a	1989 ^a	% change 1988-87
Ocean sciences	\$ 133.6	\$ 124.1	\$ 121.3	10%
Physics	126.6	118.6	115.8	7
Materials research	117.4	109.7	107.0	7
Chemistry	101.0	89.8	87.8	13
Atmospheric sciences	100.6	96.8	95.0	4
Astronomical sciences	85.1	84.2	82.8	1
Molecular biology	67.1	62.0	60.9	8
Biotic systems and resources	66.5	61.0	58.1	9
Mathematical sciences	59.8	51.7	47.7	16
Cellular biology	56.6	52.1	52.4	9
Earth sciences	55.0	49.0	45.9	12
Behavioral, neural sciences	48.9	45.7	44.4	7
Computer research	44.5	40.2	39.1	11
Social and economic sciences	31.4	30.0	28.8	5
Information and science technology	11.9	9.3	8.9	28
TOTAL	\$1108.0	\$1024.2	\$995.7	8%

a Estimate. b Actual. Source: National Science Foundation

. . . and for chemical programs

\$ Millions	1987 ^a	1988 ^a	1989 ^a	% change 1988-87
Chemistry	\$101.0	\$ 89.9	\$ 87.6	13%
Chemical dynamics	17.6	16.0	15.5	10
Structural chemistry and thermodynamics	17.1	15.5	15.0	10
Chemical physics	16.6	14.9	14.4	11
Chemical instrumentation	14.1	11.6	11.6	22
Chemical analysis	12.5	11.3	11.1	11
Synthetic organic, natural products chemistry	12.3	10.9	10.6	13
Synthetic inorganic, organometallic chemistry	10.6	9.5	9.3	12
Materials research	57.4	55.8	55.9	3
Laboratories	27.7	27.2	27.1	2
Solid-state chemistry	9.1	8.7	8.2	5
Polymers	7.5	7.1	7.6	6
Ceramics and electronic materials	6.9	6.6	6.5	5
Instrumentation	6.2	6.2	6.5	—
Chemical, biochemical, and thermal engineering	30.1	29.1	29.1	3
Thermal systems	9.0	8.5	8.8	6
Thermodynamics, transport phenomena	4.7	4.6	4.5	2
Process and reaction engineering	3.7	3.4	3.5	9
Multiphase, interfacial phenomena	3.6	3.4	3.3	6
Kinetics and catalysis engineering	3.3	3.1	3.0	6
Separation and purification processes	3.2	3.1	2.9	3
Biochemical and biomass engineering	2.6	3.0	3.1	-13
Biochemistry	16.1	15.1	14.0	7
Chemical oceanography	13.3	12.8	12.4	6
Geochemistry	10.0	9.7	9.7	3
Atmospheric chemistry	9.2	7.3	7.1	26
TOTAL	\$237.1	\$219.5	\$215.8	8%

a Estimate. b Actual. Source: National Science Foundation

Administration still trying to cut NIH budget

\$ Millions	1987 ^a	1988 ^a	1989 ^a	% change 1988-87
National Institutes	\$4589.6	\$4987.1	\$4720.9	-8%
Cancer	1158.1	1252.7	1186.8	-8
Heart, Lung & Blood	785.7	859.2	805.3	-9
General Medical Sciences	471.5	514.8	482.3	-6
Diabetes & Digestive & Kidney Diseases	419.0 ^c	569.3	543.6	-26
Neurological & Communicative Disorders & Stroke	399.4	433.4	396.9	-8
Allergy & Infectious Diseases	330.6	383.5	371.0	-14
Child Health & Human Development	309.1	321.8	313.3	-4
Environmental Health Sciences	188.0	197.5	194.8	-5
Eye	179.2	195.1	181.7	-8
Aging	145.8	156.5	144.5	-7
Arthritis & Musculoskeletal & Skin Diseases	106.7	—	—	—
Dental Research	96.5	103.3	100.7	-7
Research resources	234.2	305.7	304.0	-23
National Library of Medicine	56.4	57.8	55.9	-2
John E. Fogarty Center	11.3	11.8	11.7	-3
Research facilities	8.0	14.9	21.7	-46
TOTAL	\$4899.5	\$5377.1	\$5114.2	-9%

a Estimate. b Actual. c Funding is low because of new institute for arthritis. Source: Office of Management & Budget

Defense research posts another big gain

\$ Millions	1987 ^a	1986 ^a	1985 ^b	% change 1986-87
Tactical programs	\$12,671.5	\$10,901.0	\$ 9,062.2	16%
Strategic programs	9,429.6	8,054.4	8,169.0	17
Advanced technology development	6,574.7	4,234.3	2,750.6	55
Intelligence and communications	5,102.9	4,703.4	3,953.0	9
Program management and support	4,566.0	4,124.5	3,814.0	11
Technology base	3,585.3	3,449.0	3,120.7	4
TOTAL	\$41,930.0	\$35,475.6	\$30,869.5	18%

^a Estimate. ^b Actual. Source: Department of Defense

Agricultural research is down slightly

\$ Millions	1987 ^a	1986 ^a	1985 ^b	% change 1986-87
Agricultural Research Service	\$515.0	\$486.2	\$516.6	6%
Cooperative State Research Service	246.3	278.9	304.3	-12
Forest Service research	111.5	120.1	121.7	-7
National Agricultural Library	11.4	10.8	11.4	6
TOTAL	\$884.2	\$896.0	\$954.0	-1%

^a Estimate. ^b Actual. Source: Department of Agriculture

Big loss for EPA research wipes out '86 gains

\$ Millions	1987 ^a	1986 ^a	1985 ^b	% change 1986-87
Air	\$ 63.2	\$ 68.4	\$ 66.4	-7%
Energy/acid rain	59.6	59.1	56.8	1
Hazardous waste	50.6	51.8	46.6	-2
Toxic substances	32.4	34.9	25.0	-7
Water quality	24.4	27.7	27.3	-12
Drinking water	22.5	24.2	23.3	-7
Interdisciplinary	19.4	24.6	26.6	-21
Pesticides	13.2	11.8	9.7	12
Management/support	9.7	9.3	9.5	4
Radiation	0.2	0.2	1.9	0
Superfund	c	12.6	12.4	—
TOTAL	\$295.2	\$324.6	\$305.5	-9%

^a Estimate. ^b Actual. ^c No Superfund R&D budget for 1987. Source: Environmental Protection Agency

NASA's R&D funding continues to climb

\$ Millions	1987 ^a	1986 ^a	1985 ^b	% change 1986-87
Conduct of R&D	\$3003.1	\$2756.8	\$2468.1	9%
Physics and astronomy	539.4	607.1	677.2	-11
Space applications	526.6	518.7	374.1	2
Space transportation	465.5	437.0	391.4	7
Space station	410.0	205.0	155.5	100
Aeronautical research	376.0	354.0	342.4	6
Planetary exploration	323.3	352.8	290.9	-8
Space research & technology	180.2	168.0	150.0	7
Life sciences	74.7	69.9	62.3	7
Commercial programs	45.3	28.1	9.5	61
Transatmospheric research	45.0	—	—	—
Tracking & data acquisition	17.1	16.2	14.8	6
R&D facilities	181.3	139.3	157.6	30
TOTAL	\$3184.4	\$2896.1	\$2625.7	10%

^a Estimate. ^b Actual. Source: National Aeronautics & Space Administration

A number of major NASA programs have been cut back substantially in the 1987 proposal. Among them are the gamma-ray observatory, down 41% to \$55 million; the Hubble space telescope program, down nearly 80% to \$28 million; and the Venus radar mapper mission, down 47% to \$67 million. However, there would be some large increases in the areas of data and research analysis and in the Mars observer project, which would get a funding increase of 66% to \$63 million.

The total figure for federal nondefense R&D stays barely even; but the National Science Foundation's 1987 budget leaps a full 8%—from \$1.56 billion to \$1.69 billion. Even so, NSF director Erich Bloch insists the \$130 million rise is "a modest increase, given the needs of the country."

Chemistry fares well in the proposal, with funding rising 13% to \$101 million, and funding for the closely related field of materials research rising 7% to \$117 million. The foundation's engineering research program continues to receive strong emphasis with a 14% jump to \$186 million. Bloch isn't specific, but he says three to five more of the vaunted Engineering Research Centers would be funded in 1987. That comes somewhat as a surprise, since prebudget rumors held that no more than two would be funded.

Bloch points out that NSF is emphasizing four areas of growth in its 1987 plans:

- Biotechnology, funding for which rises from \$86.5 million to \$106.5 million and will include a series of large and small centers of specialty.

- Computational science and engineering, funding for which rises from \$57 million to \$84 million, to build upon the supercomputer revolution sweeping basic science and engineering today.

- Global geosciences, funding for which increases from \$17.6 million to \$35.6 million, as part of an interagency push to understand natural disasters better and to study the impact of technology on natural processes.

- "Broadening participation in science and engineering research and education" to further bring women and minorities into the scientific mainstream and beef up the scientific capabilities of small colleges.

No new supercomputer centers will be established, Bloch says, but the \$54 million budgeted for advanced scientific computing will go toward linking up computer facilities of all types and maintaining the five big centers that already are being established with funds from the current fiscal 1986 budget.

He adds that support for instrumentation and facilities will be increased across the board. "In chemistry, increased support for shared instrumentation will be provided," he says. Broken out as a line item for the first time in this year's budget proposal, funding for chemical instrumentation is up 22% to \$14.1 million.

For the Department of Agriculture, the Administration request is less than 1% below the 1986 budget, after the deficit reduction cuts are made. Funding for USDA's primary research organization, the Agricultural Research Service, would increase \$29 million to

\$515 million. The increase would provide additional funds for research into new food and more nonfood uses of agricultural products. More than \$3 million would go to research on plant germplasm, which follows a recent move to put more emphasis on biotechnology in agriculture.

The Cooperative State Research Service, which manages funds for research at state agricultural experiment stations and other institutions, would get a 12% funding cut. That comes on top of the 1986 Gramm-Rudman-Hollings reductions. About the only good news for the office's programs is a \$6.7 million increase in funding for the experiment stations and \$1 million more for the predominately black colleges set up in 1890 and Tuskegee Institute. The special research grants program and the animal health and disease program are to be eliminated. In addition, two training grant programs, the Morrill-Nelson and the Competitive Graduate Training Grants, are to be cut drastically or eliminated because the Administration believes they are not needed.

Forest research would be trimmed nearly 7% to \$112 million in 1987. USDA says two programs, a \$6.5 million competitive grants program and an acid precipitation survey, account for the drop.

Also on the down side is the Department of Interior's R&D budget, down 10%, or \$36 million, to \$345 million. The budget for the Geological Survey, which accounts for about 90% of Interior's R&D funding, would decline \$14 million to \$204 million. The Bureau of Mines' R&D budget would drop \$22 million to \$61 million. The Administration is proposing to eliminate the federal contribution to the mineral institutes, which support minerals research and engineering programs, at 31 colleges and universities. Research obligations for the Fish & Wildlife Service, which among other things studies the impact of broad-scale environmental changes on fish and wildlife populations and habitat, would be held essentially constant at \$49 million.

The Administration proposes a fairly drastic reduction of 28% in the Department of Commerce's R&D programs. At the National Oceanic & Atmospheric Administration, R&D obligations would decrease 25% from 1986 to \$192 million. According to OMB, the Administration wants to do away with "lower-priority" research in such programs as Seafloor Spreading Center Research, National Underseas Research Program, National Sea Grant College Program, and some programs of the National Marine Fisheries Service. A 1986 rescission proposal of \$28.9 million in the Sea Grant program accompanied the new budget to Capitol Hill. However, NOAA is expected to increase its research on radiatively important trace species and hurricane predictions, while maintaining its acid rain research program.

The proposed overall budget for the National Bureau of Standards is down just 3%, or \$5 million, to \$121.8 million. However, its operating budget, which supports its research activities, would decline 10%, or \$12 million, to \$111.3 million. The budget includes funds for construction of the new cold neutron re-

search facility used for materials science. However, for what seems like the umpteenth year in a row, the Administration is proposing to do away with the Center for Fire Research and the Center for Building Technology. This year it has added the technical competence program, the computer sciences and technology program, and the research associates program to the list of programs to be eliminated or reduced.

The R&D budget at the Environmental Protection Agency is one of the smallest in the federal government, but because its results are a base for all-encompassing regulations, it is watched carefully. For 1987, the Administration is proposing a 9% decrease in EPA's R&D budget to \$295 million. Major cuts are planned in the areas of water quality, down 12%, and interdisciplinary research, down 21%. It is mainly exploratory research—that is, research not tagged to specific problems—that is being cut.

Another reason for the drop is the loss of the Superfund research program. Because Congress has not yet passed a reauthorization bill for Superfund, the Administration has made no R&D request for it. If one were there, something in the range of \$13 million might be proposed. A research program is included in the bill now being considered by a House-Senate conference committee. Extramural research contracts under Superfund are starting to expire, and that is one of the reasons EPA Administrator Lee Thomas has asked for interim Superfund money.

The only program areas with some increase in support are acid rain, still a problem looking for a solution; and pesticide research, which is being expanded to accommodate more recombinant DNA and ecological studies.

The agency says that expanded cross-media research is being supported, and it mentions the problem of air emissions from uncontrolled hazardous waste dumps as an area needing more attention. Two other areas mentioned are research to support the new air toxics strategy and work to get a better determination of pesticide contamination of groundwater.

In another area, one program that was scheduled for elimination in the 1986 budget request—Tennessee Valley Authority's fertilizer development center in Muscle Shoals, Ala.—is alive, if not exuberantly healthy, in the 1987 budget request. That facility's budget would decline 16% to \$48.5 million. And the Administration intends for the facility's technology development work to become self-supporting in 1987.

In the years before Gramm-Rudman-Hollings, the Reagan budget proposals could pretty much be viewed as a floor through which the R&D budget would not fall. When the Administration asked for decreases in the NIH budget, or the fossil energy R&D program, or EPA's R&D budget, the Congressional response was to at least increase the request. The one exception has been the DOD R&D budget, for which Congress has normally cut back what would have been very large increases. That pattern may well hold true again this year. R&D makes up such a small part of the total federal budget, just 6%, that cutting it drastically isn't going to result in any noticeable savings. □

Natural Gas-Based Chemicals Pressured by Imports

Operating rates sag as imports of ammonia, urea, and methanol from countries with lower-cost feedstocks continue to increase

Bruce F. Greek, C&EN Houston

In spite of lower production costs resulting from declining natural gas prices, producers of ammonia, urea, and methanol expect to fill a smaller part of total U.S. demand this year and for the rest of this decade. Makers of these natural gas-based chemicals are joining the ranks of some other manufacturers, such as the auto and textile industries, whose plant operating rates are sagging although demand is holding.

Demand for ammonia and urea is forecast to decline slightly this year because of farm economic woes. However, demand is expected to decline less than production. Methanol's demand and production is

expected to rise in 1986. However, output of none of these three will match demand, so imports will continue to play an important role. In the case of methanol, imports will account for more than 25% of supply.

The increase in imports of ammonia, urea, and methanol results in part from the lower prices offered by countries with lower feedstock (specifically methane) costs.

Key Chemicals

Some sizable quantities of these materials come from areas, including communist countries, where U.S. companies have no influence on production other than a willingness to bargain on purchase prices. This shift has occurred even as U.S. natural gas prices weakened slightly and then began to decline more steeply. The trend toward increas-

ing imports is not expected to reverse anytime soon. Even with further reduction in U.S. natural gas prices, the differential between this country's gas costs and foreign gas costs in such areas as Canada and Trinidad will stay relatively large.

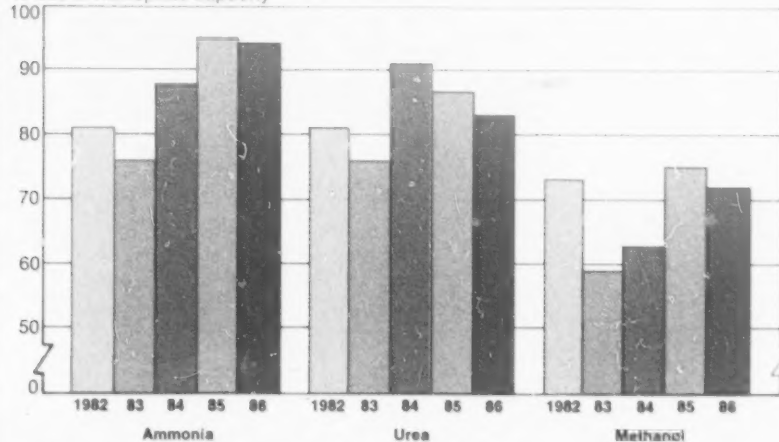
Significant imports of gas-based chemicals, accounting for an important part of U.S. demand, will continue for years even as domestic natural gas costs decline. Although those prices will decline less than have crude oil prices recently, they will continue to fall as market competition forces natural gas producers to reduce selling prices. Generally, industrial natural gas's major competitor is residual fuel oil. Both are used heavily in power generation, in addition to coal and nuclear fuel. Power plant operators have found it economically desirable to build in flexibility to use either natural gas or oil. During the past five years, this flexibility has been pursued widely. Therefore, as crude oil prices decline, pressure will continue on natural gas prices. As a result, about two thirds of cash production costs (made up of gas for feedstock and fuel) for ammonia and methanol will decline more rapidly than all other costs, including capitalization.

With lower natural gas prices, ammonia and methanol producers would temporarily enjoy lower costs, and possibly a respite from further loss of markets to importers whose costs for all but feedstock and fuel continue to rise. However, as the lower-cost gas is consumed over the next few years, these chemical producers may face declining supplies unless prices reverse their current trend.

For details of the near-term outlook for ammonia, urea, and methanol, please see the following pages.

Capacity use dropping this year

% use of nameplate capacity



Sources: International Trade Commission, Census Bureau, C&EN estimates

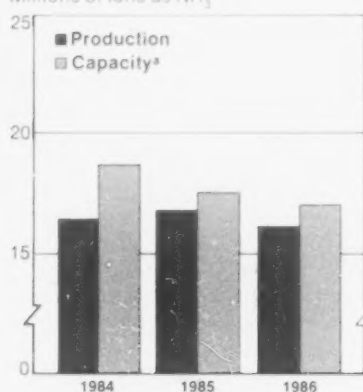
Ammonia



- **Production to fall**
- **Capacity down**
- **Prices lower**

PRODUCTION/CAPACITY

Millions of tons as NH_3



■ First quarter, some capacity idled.

MAJOR PRODUCERS

CF Industries, Chevron, Farmland, Union Oil, Williams Cos. (Agrico)

HOW MADE

Catalytic reaction of nitrogen from air and hydrogen from natural gas

MAJOR DERIVATIVES

Ammonium nitrate 20%, urea 20%, ammonium phosphates 15%

MAJOR END USES

Fertilizers 80%, fibers and plastics 10%, explosives 5%

FOREIGN TRADE

Exports—falling to about 500,000 tons, imports—falling to about 2.5 million tons

PRICES

About \$110 per ton on Gulf Coast

U.S. production and consumption of ammonia almost certainly will fall in 1986. The key question is how much production will decline—and that could differ significantly from the expected decrease in consumption.

Current forecasts, in this early part of the fertilization and growing season, call for U.S. ammonia output to decrease only modestly to 16 million tons, about 4% less than 16.6 million tons estimated for 1985. That will account for less than 90% of anticipated consumption. The net of imports of ammonia over exports of some 2 million tons will supply nearly all the remainder of demand. Inventory changes are expected to be minimal in 1986.

Consumption of ammonia this year probably will exceed 18 million tons, with more than 80% going either directly as fertilizer or made into other forms of nitrogenous fertilizer, such as urea, ammonium nitrate, or diammonium phosphate. Large and unpredictable quantities of these other forms of nitrogen-containing fertilizers also will be exported. Sometimes in the past, direct exports of ammonia and exports of nitrogen fertilizers have accounted for nearly a quarter of ammonia consumption. On the basis of total change in ammonia equivalents, the net of exports less imports will be lower in 1986 than it was in 1985.

Total ammonia consumption expected in 1986 in the U.S. will be down more than will production, probably in the range of 6%, or about 1 million tons. Agricultural uses will be down even more, possibly as much as 10%, but more likely 8%, when the final results of reductions in crop acreage are determined. In 1986, exports of some nitrogen fertilizers could increase modestly as a result of a decline in the strength of the dollar and because of lower selling prices. Imports of ammonia and derivatives likely will decline as well, because lower selling prices for ammonia are expected to hold during most of the year.

Consumption of ammonia (as well

as of other fertilizers) will depend on variables other than weather. For example, the financial condition of agriculture in general is worse than it has been in recent years. It's questionable whether 10 to 25% of farmers will be able to pay for or to get loans to buy fertilizer they need.

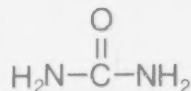
New farm legislation is attempting to make U.S. agricultural products more competitive in world markets. Farm crop support prices are expected to be lowered, but it is hoped that farm income will be maintained. That could loom large in fertilizer consumption.

As part of the effort to reduce surpluses, various programs to reduce planted acreage have been proposed. Some of the proposals call for up to 90 million acres to be taken out of the total 340 million acres planted in 1985. Sources suggest that nearer 30 million acres will be left unplanted, which is less than a 10% reduction. Farmers likely will not plant the poorer land and will more heavily fertilize the better land to increase yields, suggesting a slightly improved use of plant nutrients per acre for 1986.

Nonagricultural uses of ammonia account for less than 20% of U.S. consumption. Such uses, the largest of which are in making intermediates for major-volume fibers such as acrylonitrile and nylons and as blasting agents, are barely growing.

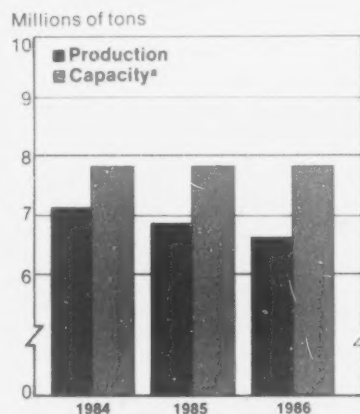
Ammonia producers and importers will easily supply the 1986 demand except during the peak month of April, a month when a distribution problem regularly occurs. New ammonia capacity recently completed in Canada will supply material at prices competitive with the now reduced U.S. production costs. Additional U.S. ammonia capacity may be shut down, following the 1.5 million tons of capacity closed over the past two years. However, the U.S. ammonia industry has finally become very lean with the forecast average plant operating rate for 1986 at more than 90% of nameplate capacity.

Urea



- **Production to slow**
- **Capacity on hold**
- **Prices weak**

PRODUCTION/CAPACITY



MAJOR PRODUCERS

CF Industries, Farmland Industries, Triad, Unocal, Williams Cos. (Agrico)

HOW MADE

Reaction of ammonia and carbon dioxide under pressure

MAJOR DERIVATIVES

Urea-formaldehyde resins 5%

MAJOR END USES

Fertilizers 80%, animal feeds 10%, adhesives and plastics 5%

FOREIGN TRADE

Exports—falling below 1 million tons, imports—declining below 2 million tons

PRICES

About \$100 per ton on Gulf Coast

Urea production outstripped forecasts in 1984 and 1985 because of strong U.S. demand. And it could surprise forecasters this year, too.

However, it's unlikely that strong demand for urea will push production this year above that in 1985. Present forecasts, made before the major consumption rush begins in April, are for a 4% decline from 1985 to 6.5 million tons. Production in 1985, estimated at more than 6.8 million tons, also was down from the previous year's 7.15 million tons, which was close to the all-time high of about 7.5 million tons in 1981.

There's no mystery why demand for urea is expected to be down this year—lower U.S. demand for nitrogenous fertilizers and animal feeds, smaller exports, and little, if any, change in demand for urea formaldehyde resins and other miscellaneous nonfarm uses. Imports of urea may increase slightly to reduce U.S. production, but current low selling prices and relatively high inventories will tend to hold down imports.

Total demand for urea of about 7.4 million tons in 1986 likely will exceed U.S. production about 750,000 tons. That amount will be met by a combination of imports from traditional suppliers such as Canada and Western Europe, from other sources such as the U.S.S.R. and Eastern Europe, and from the result of barter deals involving grain. Total demand will be down about 7.5% from the recent high of slightly more than 8 million tons a year.

In the U.S., agricultural demand for urea will be affected by weather and farming economics, but export demand also could upset forecasts. Some past major importers of urea such as China and India at times dropped out of the market in 1985, cutting U.S. exports drastically. Even with a decline in the value of the dollar, other countries—Indonesia for one—could capture a part of U.S. export markets as those countries bring on new capacity and

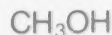
seek to replace declining revenues from sale of petroleum and natural gas. Nevertheless, former large importers of U.S. urea could end up requiring more material than they can obtain from other countries, and again may buy U.S. product, resulting in low forecasts.

Weather and distribution limits might upset demand forecasts, because of a growing acceptance of solutions of urea and ammonium nitrate (UAN solutions) as a nitrogenous plant nutrient. If the weather is good in April and May when very large amounts of ammonia are applied to cornfields, local demand could exceed supplies available for immediate application. (Corn requires about 40% of nitrogen fertilizers in the U.S.)

Moreover, farmers might encounter delays in financing fertilizers at this time, resulting in a significant amount of cropland's receiving less nitrogen than desirable. To make up for this kind of deficiency, farmers could "side dress," which means apply UAN solution between the crop rows after corn is several inches high. In that case, the demand would surge a few months after normal fertilization time, raising consumption of urea unexpectedly high near the end of the fertilizer year.

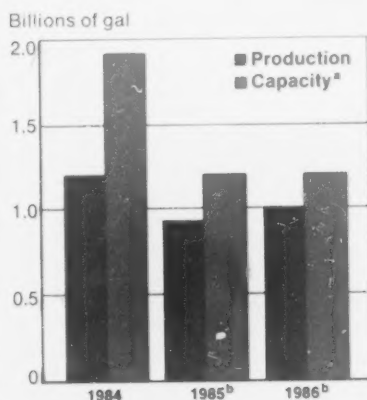
Complex economics also enter into demand for urea. Currently, urea has two major price areas. High-quality, well-formed urea granules bring \$100 to \$110 per ton on the Gulf Coast. Dusty, off-grade urea (often imported material) sells for about \$85 per ton. The high-quality material sells well because of the ease with which it can be made into solid mixed fertilizers. The dusty material will go to make UAN solutions, which, because of handling expenses, eventually will cost the user about the same as high-quality urea. If demand for UAN solutions for later side dressing is strong, then imports could rise, supplementing strained production plants late this spring and selling for better prices because all grades of urea might cost more.

Methanol



- **Production down**
- **Capacity in flux**
- **Prices holding**

PRODUCTION/CAPACITY



a First quarter. b Additional 700-plus gal of capacity on standby

MAJOR PRODUCERS

Arco Chemical, Borden, Celanese, Du Pont, Texaco

HOW MADE

Reaction of carbon monoxide and hydrogen made by reforming natural gas (methane), and heavier hydrocarbons; gasification of coal

MAJOR DERIVATIVES

Formaldehyde 30%, acetic acid 10%, chloromethanes 10%

MAJOR END USES

Polymers used as adhesives, fibers, and plastics 50%; fuels and fuel components 20%

FOREIGN TRADE

Exports—declining further to less than 10 million gal, imports—leveling off at about 400 million gal

PRICES

About 40 cents per gal in volume

Synthetic methanol production in the U.S. will grow significantly during 1986, and operating capacity will increase, but only temporarily. That outlook suggests that producers might have better business prospects now than they had in the past two years. About a third of U.S. capacity was shut down during that time, and imports soared to meet nearly a quarter of demand. Meanwhile, exports dwindled to almost nothing.

The recovery, however, remains relative. Plans for restarting shuttered capacity depend on the economics of the industry rather than upon those of a single plant. Consumption of methanol in the U.S. is expected to increase very little this year, if the economy remains near its present growth rate. Manufacturing costs and selling prices are trending downward, with still much concern about whether costs can continue dropping faster than prices.

Operating capacity is expected to shift some this year. Probably no later than early in the second quarter, Du Pont will have completed restarting its methanol unit at Beaumont, Tex. With a capacity of 250 million gal a year, the Beaumont unit will more than replace the 200 million gal of capacity at Deer Park, Tex., which Du Pont will close as part of its plan to end, by 1987, its Syngas Co. joint venture with the USI division of National Distillers & Chemicals.

Using residual fuel oil, the Syngas plant makes synthesis gas—carbon monoxide and hydrogen—from which Du Pont makes methanol and USI makes acetic acid. The Du Pont-USI agreement for ending the partnership calls for Du Pont to modify the synthesis gas plant so that USI can assume ownership and operation of it. Du Pont also will withdraw from methanol production at that plant, after shutting it down late in 1986.

If the startup of the Beaumont unit goes smoothly, Du Pont probably will be able to produce at least 150 million gal of methanol at the unit during 1986.

This capacity startup will account for most of the estimated increase in total U.S. methanol production in 1986, an increase to more than 1 billion gal, about 10% more than in 1985.

As a result of Du Pont's startup, capacity at the beginning of 1987 will be close to that at the beginning of this year, unless other capacity changes occur this year as a result of oil and gas price declines that have already begun. For 1986, actual operating capacity to make methanol will total about 1.4 billion gal. Without other changes in capacity, with imports at no more than 400 million gal, and with demand totaling 1.4 billion gal, the average plant operating rate this year will be about the same as last year's, 70 to 75% of nameplate capacity.

At about 1.4 billion gal, methanol demand will be up only marginally from last year's, fitting the pattern of smaller and smaller growth rates in recent years. As in the past few years, much of the growth this year will come from two uses—fuels and acetic acid. If housing and commercial construction follows optimistic forecasts and holds at last year's rates or increases, then methanol's major use—in formaldehyde—will increase slightly. However, formaldehyde's share of consumption of methanol likely will decline again because of faster growth of other uses. Resins and resin intermediates account for about 90% of formaldehyde consumption, with the two big resins, urea- and phenol-formaldehydes, taking half the total. Most of the formaldehyde-related resins are mature products with relatively low growth prospects.

The faster growing area of methanol consumption currently remains the fuel uses. With phaseout of lead additives in gasoline nearly complete, supplies of high-octane blend stocks are strained, creating strong demand for methanol-*tert*-butyl alcohol blends and methyl-*tert*-butyl ether (MTBE). In 1986, the fuel and fuel additives uses of methanol will take more than 10% of consumption.

Shortage of water fluoridation chemicals developing

David Webber, New York

Danger signals are flashing for supplies of the chemicals most commonly used to fluoridate municipal drinking water. Suppliers and government experts consider a shortage of the compounds, which are key to municipal programs to reduce tooth decay through treatment of water supplies, to be imminent. Reason: the agricultural slump.

It might seem a long distance from corn belt woes to municipal water systems, but supply of fluoridation chemicals is entirely dependent on the farm economy. The three major fluoridation compounds—hydrofluosilicic acid (HFSA), sodium silicofluoride (SSF), and sodium fluoride—are largely by-products of phosphoric acid production. No one produces the fluoridation chemicals on purpose. But phosphoric acid production has essentially come to a halt since Christmas, because inventories of derivative fertilizer products are overabundant.

As a result, say fluoridation chemical distributors, supply of HFSA and SSF, the two most popular compounds, has slowed to a trickle. HFSA "has been in extremely short supply since December, and it is getting worse," says Richard J. Lucier of LCI, Clayton, Mo., one of the major suppliers of the fluoridation chemicals bought under contract by community water systems in the U.S. (Chemtech is another major distributor.) Lucier has notified customers that he will soon begin allocating deliveries.

Thomas G. Reeves, national fluoridation engineer at the Centers for Disease Control (CDC) outside Atlanta, confirms the supply problem. "Supplies are tight now in most places and, in a few incidences, have run out or are about to," he comments. Reports coming into CDC, the lead agency in the nation's water fluoridation effort, so far have pinpointed spot shortages in Baltimore, several communities in Ohio, and parts of Louisiana, according to Reeves. "It looks like we will have a shortage," he says.

Observers believe the current

tightness will become a real shortage because there is little sign that the fertilizer industry is about to recover anytime soon. "Any pickup in production is very unlikely in the near future, given the demand outlook for fertilizer by U.S. agriculture during the current crop year and given the depressed state of the export market," remarks Donald N. Collins, a Fertilizer Institute spokesman. Last month, the European Economic Community, in retaliation for U.S. quotas on EEC steel exports to the U.S., imposed similar restrictions on exports of finished phosphate fertilizers from the U.S. to EEC countries. "Although the tonnage is not large, it's another dent in U.S. exports," Collins says.

Another negative is the nature of phosphate fertilizer use. Unlike nitrogen-based fertilizers, which must be applied each season, phosphate fertilizers are not so essential. Farmers can skip a few applications, and they did so last fall. There is little reason to expect that cash-strapped farmers will buy any more phosphate fertilizer this spring than they absolutely must.

The difficulty in ensuring an unbroken adequacy of supply of the major water fluoridation chemicals stems not only from their being by-products, but because recovering and purifying them to water-treatment grade is not particularly lucrative. Collection units are expensive to buy, and they are expensive to maintain because of heavy scaling. The bulk of the HFSA recovered, for instance, is discharged into settling ponds or, when permitted, into local waterways. Very little was even recovered from stack gases before Environmental Protection Agency regulations began requiring it in the early 1970s.

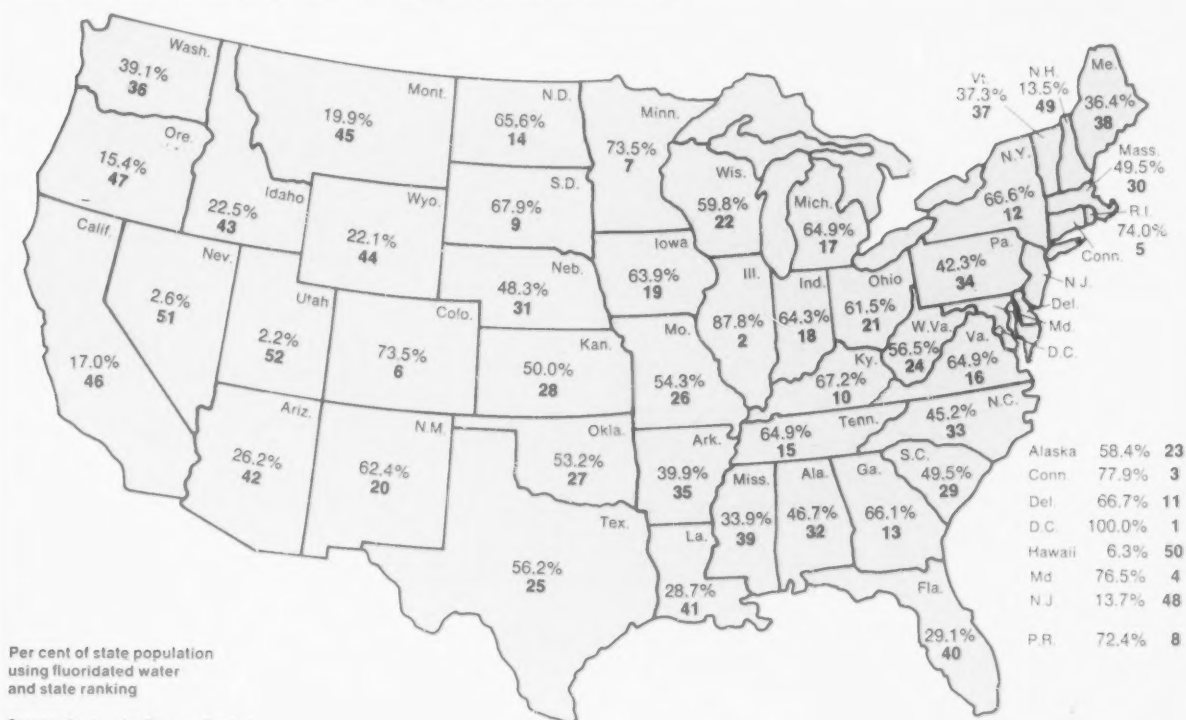
It was air pollution control regulations, in fact, that resulted in bulk collection of HFSA, now by far the most commonly used fluoridation chemical. The reason is cost: HFSA sells to the biggest municipalities for about 4 cents per lb and to smaller communities for 15 to 20 cents per lb. By comparison, SSF sells for 25 to 30 cents per lb, and sodium

fluoride for an average of 85 cents per lb, according to CDC's Reeves. It takes 46 lb of HFSA to bring 1 million gal of water to 1 ppm fluoride. Because the yield of fluoride ion per unit varies, it takes only 14 lb of SSF and 19 lb of sodium fluoride to accomplish the same task, Reeves explains. But HFSA is still the product of choice on price considerations: \$1.84 for a large city to bring each 1 million gal to 1 ppm fluoride, compared to \$3.85 for SSF and \$16.15 for sodium fluoride.

Communities do not decide which compound to use solely on the basis of chemical cost, however. For one thing, HFSA is sold in solution (typically 25% acid to 75% water), requiring expensive solution metering pumps, storage tanks, and other bulk handling facilities. Communities with less money to spend often choose SSF, which can be added to the water supply through a dry feeder, still a big piece of equipment. Only the smallest systems, in general, use the expensive sodium fluoride, which can be administered via a saturator, the least costly equipment possible. Also, handling liquid HFSA can be hazardous, whereas SSF and sodium fluoride, as powders, are safer. That can be another key consideration to smaller communities that cannot afford extensive safety precautions.

What bothers people at CDC, the National Institutes of Health's National Institute of Dental Research, and other agencies about the current supply situation is that it is recurring. There was a two-month shortage in 1982 and several others in previous years. "What concerns me is the pattern of shortages," points out fluoridation expert Reeves. "They tend to come more closely together, and they tend to be more severe every time. If this one is more severe, it would continue that pattern." And there is good reason to expect the pattern to continue: At CDC urging, more communities are beginning to fluoridate their drinking water supply. Most of them use HFSA. Second, long-term trends, such as the decline of agricultural export markets and the rise of for-

Only 54% of U.S. population uses fluoridated water



eign phosphate fertilizer industries, spell continued difficulties for U.S. fertilizer production.

Still, the problem is not by-product capacity. Just a few of the phosphoric acid plants could easily supply all the HFSA needed in the U.S. to both municipal water systems and the aluminum industry, the other major consumer. The problem is the periodic gaps in production coupled with a lack of storage capacity. Because the water content of HFSA solution is so high, enormous tank facilities would be required to hold enough acid for more than just a few weeks' supply. But very few municipalities are likely to spend the money on tank farms. As it is, distributors complain that community purchasers will change suppliers on the basis of a marginally lower bid from a competitor. Nor are fertilizer producers interested in building storage capacity for a pesky by-product.

Reeves believes that the installation of storage capacity could be encouraged by state legislatures through either direct funding or tax breaks. The problem with that solu-

tion, he concedes, is getting state officials, who are the ones with the authority in the fluoridation effort, interested enough. "I have talked about it with state people," Reeves says, "but nothing has ever been done. The trouble is that nobody's really concerned until there's a shortage, and then it's too late."

"At CDC, we've been urging communities to have more on hand. We get a mixed reaction. Some listen if they're in a state with a good state fluoridation engineer tend not to listen to us."

A shortage of fluorine compounds could become serious, studies have shown, if drinking water devoid of tooth-decay-fighting fluoride is consumed for a month or so, however, municipal governments would need to consider alerting dentists to the problem. Dentists could then prescribe fluoride tablets or drops to children, something that is now done regularly in many areas in which drinking wa-

ter is not fluoridated. Fluoridated toothpaste is much less effective than fluoridated drinking water.

What worries fluoridation proponents about the pattern of chemical shortages is that shortages sometimes give communities in which opinion is divided a good excuse to drop fluoridation entirely. That holds back the already lagging effort to expand the scope of the water treatment program, which began after World War II. The government's objective has long been to have 95% of the population that is served by public water supplies drinking fluoridated water by 1990. As of last October, the total was 129 million, or about 54%. The chemical shortage does not affect about 10.5 million people in the group; their water systems deliver naturally fluoridated water. The reason for the failure to make fluoridation nearly universal in the U.S. is, as has been the case from the beginning of the effort, opposition by various groups that claim fluoridation is a communist plot and blame it for cancer, AIDS, and other scourges. □

Star Wars Funds Spur University Research

At no time since the height of the Vietnam War have university researchers been as dependent on the Department of Defense for funding as they were in 1985. The Strategic Defense Initiative program, often called Star Wars, is likely to strengthen this dependency in the future, say William Hartung and Rosy Nimroody, researchers affiliated with the New York City-based Council on Economic Priorities.

During the 1980-85 period, DOD has increased its funding for university research 89%, piling the growth in National Science Foundation funding to campuses, which was 51% over that same period. This includes funding for both basic and applied research. If only basic research funding is considered, growth in the funding figures are even more startling: a 118% increase for DOD vs. a 52% increase for NSF.

In 1985, the Pentagon's share of total federal funding for university research was 16%, up from 10% in 1980. That growth rate is nearly twice as fast as any other government source of money. And propelled by funds from the innovative science and technology program within the Pentagon's Strategic Defense Initiative Organization, that rate could reach supersonic speeds in short order. The fiscal 1985 budget for SDIO's innovative program was \$28 million. Congress has granted the program a \$96 million budget for fiscal 1986. According to John P. McTague, acting director of the Office of Science & Technology Policy, the President is asking that the program's budget be \$167 million in fiscal 1987. That rise is occurring as constraints are being placed on other funding sources.

Money from SDIO is not only bountiful but, with less red tape, it is also easier to obtain. With those attributes, SDIO's innovative science and technology program already has received more than 3000 proposals. And Congress willing, SDIO plans to let university contracts within

nine months of receiving the "white paper," or proposal. SDIO had planned to let most research contracts for fiscal 1986 by Jan. 1, for instance. But, according to an SDIO spokeswoman, "the continuing budget resolution prevented this."

Nonetheless, SDIO's innovative science and technology program has already committed \$62 million for long-term contracts (\$15 million in fiscal 1986) to support six research consortia. The money and the challenge to solve technological puzzles have attracted top-notch universities and their associated laboratories. Massachusetts Institute of Technology and its affiliated Lincoln Labs, holders of the most SDI contracts; Johns Hopkins University; Princeton University; the University of California; and the University of Illinois are just a few of the 29 universities in 16 states receiving money to research areas "of critical importance to the success of SDI."

The critical areas being investigated by the consortia are: nonnuclear space power—a \$19 million four-year program; composite materials development—a \$15 million three-year program; chemical-laser exhaust problems, spacecraft radiation, electromagnetic waves, and particle beams—a \$12.5 million three-year program; optical computing—a \$9 million three-year project; electronic circuits for computing, sensing, power generation, and directed-energy beams—a \$4 million three-year program; and high-speed electronic systems, new dielectric materials for storing power for directed-energy and kinetic-energy systems, and advanced power sources for lasers and particle beams—a \$2.5 million three-year project.

Although the head of the innovative science and technology program, James A. Ionson, has said, "Any work for SDI performed on a university campus will not be classified and ... subject to any control

DOD generously funds university chemistry, chemical engineering

% funding increase, 1980-85	Chemistry	Chemical engineering
BASIC RESEARCH		
Total federal funding	65%	59%
Defense Department	127	(-80)
funding		
National Science	79	85
Foundation		
APPLIED RESEARCH		
Total federal funding	13	67
Defense Department	50	134
funding		
National Science	200	873
Foundation		

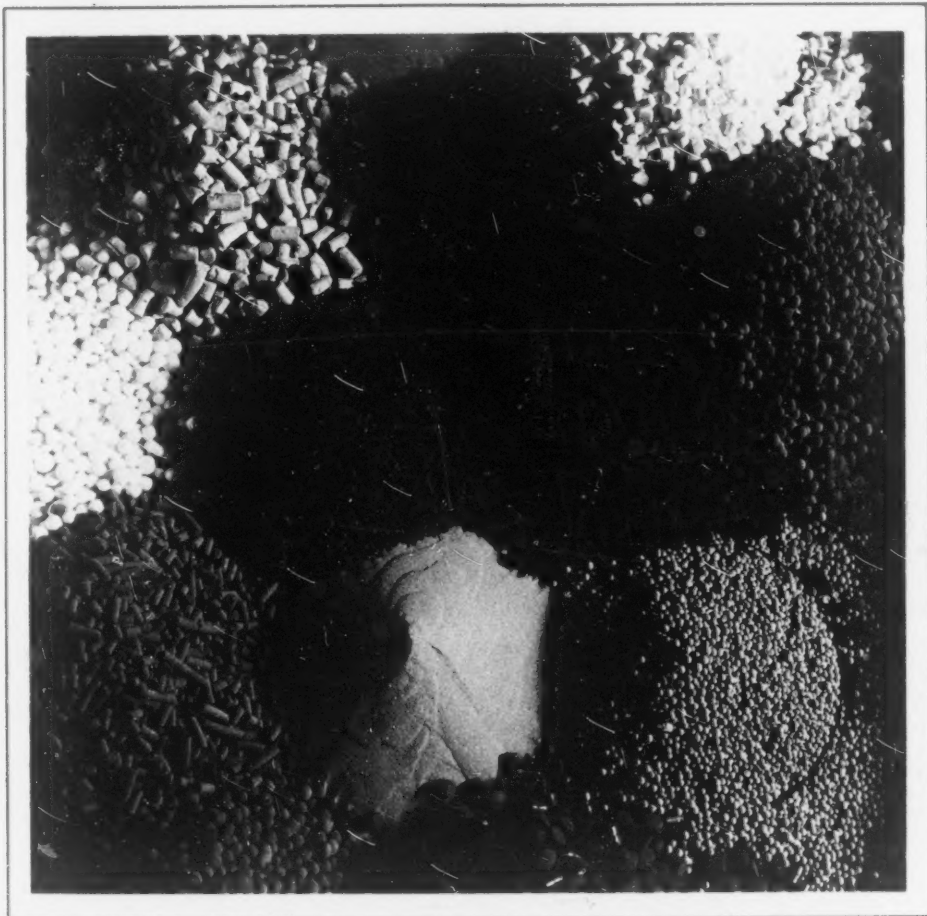
Source: Rosy Nimroody, Council on Economic Priorities, using NSF figures

or restrictive clauses or security classifications," qualms remain. The fear is that eventually the secrecy surrounding SDI will constrain academic freedom to publish and disseminate research findings. That fear has compelled more than 2100 faculty members at 43 major research institutions to pledge not to accept research funds.

As Hartung and Nimroody write in their recent report, "Pentagon Invades Academia": "The phenomenal growth of DOD university funding in general, and the SDI innovative science program in particular, threatens the diversity of funding sources and the open research process—essential strengths of scientific research at U.S. universities."

In response to a C&EN query, the SDIO office said: "SDI's innovative science and technology (IST) program spent only \$14 million at campuses last year. For fiscal 1986 we anticipate spending about \$50 million at campuses, an average of less than \$1 million per participating campus. This represents less than 1% of total government funding at universities. All IST research is open on campuses. Also, IST has over 30 research topics, which represents a wide diversity."

Lois Ember, Washington



Hershaw/Hill photo

Process Catalysts Continue on Steady Course

Stephen C. Stinson, C&EN New York

Catalysts have become a large and important business in the U.S.—one marked by slow but steady growth. U.S. sales of process catalysts (those used in refining and chemical processes) reached 4.86 billion lb in 1985, valued at \$955 million. Their use is forecast to grow at an annual rate of 2% to 5.4 billion lb in 1990, worth \$1.12 billion. Those figures are based on a study of the U.S. catalyst market by the research firm Frost & Sullivan, New York, N.Y.

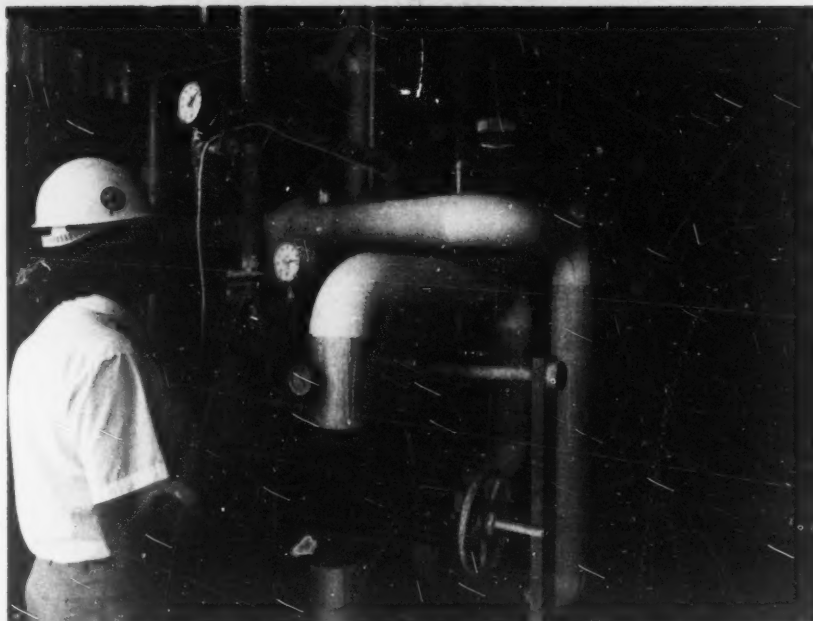
Process catalysts are used in such petroleum refining processes as al-

kylation, hydrotreating, hydrocracking, and catalytic cracking and reforming, and in such chemical processes as polymerization, alkylation, oxidation, hydrogenation, and dehydrogenation. Thus process catalysts exclude those that reduce automobile and industrial plant emissions. By custom, the field of process catalysts does include organic peroxides, however, even though they are not true catalysts but initiators of free-radical chain reactions.

As Frost & Sullivan analysts point out, the use of large volumes of commodity chemicals as catalysts

distorts any simple picture of this market. These chemicals are aluminum chloride and sulfuric, phosphoric, and hydrofluoric acids for alkylation. For example, of the 4.86 billion lb of process catalysts consumed last year in the U.S., 4.27 billion lb was sulfuric and hydrofluoric acids at refineries, and 90 million lb was phosphoric acid and aluminum chloride in chemical plants. Together, those amounted to 90% of the total volume used. Yet those chemicals were valued at only \$210 million, just 22% of the dollar value of total sales.

More than two dozen major firms



W. R. Grace's Davison Chemical division makes several different process catalysts at its Lake Charles, La., manufacturing facility

supply the U.S. market for process catalysts, excluding commodities. Each firm focuses on catalysts that fit its own technologies, which means that there is no universal catalyst company. For example, only eight companies service both the chemical and petroleum industries. Of the eight broad categories of catalytic chemical and refining processes that exclude alkylation, no company supplies catalysts for more than five. Even in the narrow spec-

trum of the four major catalytic petroleum refining processes besides alkylation, no company makes catalysts for more than three.

Catalyst producers tend to be departments or subsidiaries of larger firms. Though independent catalyst companies have started up from time to time, larger companies soon acquire them. Indeed, the most logical entry into the North American process catalyst market is by acquisition.

Among recent acquisitions, for example, Phillips Petroleum Co. purchased Aztec Chemical Co. (organic peroxides) and PureChem (aluminum alkyl-titanium halide polyolefin catalysts) from Dart & Kraft in 1982. Phillips combined the two companies into one division named Catalyst Resources.

Union Carbide, already in catalysts through its molecular sieves and ethylene oxide process, entered fluid catalytic cracking (FCC) catalysts by buying Katalistiks of Baltimore in 1984. Katalistiks itself had been founded in 1979 by EKA, Göteborg, Sweden, and English China Clays, St. Austell, England, who joined with a group of FCC veterans at Catalyst Recovery International in Baltimore to move into this dynamic field in Europe and the Americas.

On acquiring Gulf Oil Corp. in 1984, Chevron Corp. found itself in a catalyst-producing joint venture—between Gulf's Harshaw Chemical Corp. and Filtrol Corp. of Kaiser Aluminum & Chemical Co.—called Harshaw/Filtrol Partnership. Harshaw/Filtrol sells catalysts for chemical oxidations and hydrogenations, and for petroleum hydrotreating, hydrocracking, and FCC. Chevron was already a supplier of platinum-rhenium catalytic reforming catalysts.

In recent weeks, Kaiser has reorganized in defense against a hostile takeover. Though such reorganizations are frequently carried out to sell assets, Kaiser probably will keep its share of Harshaw/Filtrol. In fact, Kaiser has until 1989 to decide whether to buy Chevron's share in the joint venture.

And in 1985, Gulf Resources & Chemical Corp. sold its Lithium Corp. of America to FMC Corp. Among Lithco products are lithium and magnesium alkyls for polyolefin catalysts.

Another route into an area of the U.S. catalyst business is expansion from an existing base. For example, Katalistiks started life in the Netherlands with headquarters in Amsterdam and a plant in Delfzijl. After making successful inroads into the European FCC catalyst market, the company opened for business in the U.S. in 1982 and started up a 130

26 firms are major suppliers to U.S. catalyst market

	Chemical production ^a				Petroleum refining ^a			
	Polymerization	Oxidation	Hydrogenation	Dehydrogenation	Catalytic cracking	Hydrotreating	Hydrocracking	Catalytic reforming
Air Products								
American Cyanamid								
BASF								
Calsicat ^b								
Catalyst Resources ^c								
Davison ^d								
Engelhard								
Ethyl								
Foot Mineral ^e								
Halcon SD ^f								
Haldor Topsoe								
Harshaw/Filtrol ^g								
Katalco ^h								
Katalistiks ⁱ								
Ketjen Catalysts ^j								
Lithium Corp. ^k								
Lucidol ^l								
Monsanto								
Nouryl ^m								
Shell Chemical								
Stauffer Chemical ⁿ								
Texas Alkyls ^o								
UOP ^p								
Union Carbide								
United Catalysts ^q								
U.S. Peroxygen ^r								

^a Excludes producers of sulfuric, phosphoric, and hydrofluoric acids, aluminum trichloride, and urethane catalysts. ^b Division of Mallinckrodt. ^c Division of Phillips Chemical. ^d Division of W. R. Grace. ^e Owned 83% by Newmont Mining. ^f Subsidiary of Texas Eastern. ^g Joint venture of Kaiser Aluminum & Chemical and Chevron. ^h Joint venture of Nalco Chemical and Imperial Chemical Industries. ⁱ Subsidiary of Union Carbide. ^j Division of Akzo Chemie America. ^k Subsidiary of FMC. ^l Division of Penwalt. ^m Subsidiary of Chesebrough-Pond's. ⁿ Joint venture of Hercules and Stauffer Chemical. ^o Subsidiary of Allied-Signal. ^p Subsidiary of Sud-Chemie. ^q Division of Witco Chemical. Source: Frost & Sullivan

million lb-per-year plant in Augusta, Ga., in 1983.

Akzo Chemie America entered the FCC catalyst business in the U.S. when the Ketjen Catalysts division of the parent company Akzo, long established in Europe, opened a 90 million lb-per-year plant in Pasadena, Tex., in 1985. Among U.S. firms, PQ Corp. has started up a plant in Kansas City, Mo., to make catalyst-type zeolites. The firm had made detergent builder-type zeolites previously. PQ also had made chromium oxide-coated silica catalysts for producing high-density polyethylene by the Phillips process, as well as proprietary, silica-based oxidation catalysts. The Kansas City plant will supply zeolites to catalyst producers as well as make custom catalysts for isomerizations of xylenes and alkylations of benzene in the chemical industry and for hydrocracking, isomerization, and lube oil dewaxing at refineries.

In dollar sales, Davison Chemical division of W. R. Grace & Co., Engelhard, and Harshaw/Filtrol probably are the three largest U.S. suppliers of process catalysts. But because no firm competes exactly head-to-head with any other, estimates of which is "biggest" or which are the "top three" are of doubtful value. In addition, the concentration in precious metal catalysts by companies like Engelhard skews the dollar sales of such companies toward the high side relative to sales of producers whose catalysts use mostly minerals and base metals.

Among catalysts for chemical processes, polymerization catalysts have the greatest dollar sales and seem poised for strongest growth. Figures from Frost & Sullivan indicate that this segment was worth \$175 million in 1985, and will grow at almost 5% annually to \$220 million by 1990.

One source of change in distribution of polymerization catalyst types will be the continuing growth of linear low-density polyethylene (LLDPE), which will cut into the growth of LDPE. LLDPE uses Ziegler-Natta catalysts, which are combinations of titanium halides with aluminum and magnesium alkyls. Conventional LDPE is made mostly with *tert*-butyl peroxoate, with the

peracetate, perpivalate, perbenzoate, and perneodecanoate also used.

A second source of change will be the spread of the Montedison process for making polypropylene. Frost & Sullivan analysts speculate that this process uses aluminum alkyls supported on a metal oxide, a catalyst invented by Mitsui Petrochemical Industries. Previously, polypropylene was made by a Ziegler-Natta combination of aluminum alkyls and titanium trichloride.

Montedison and Hercules have formed a joint venture called Himont to commercialize and license the newer technology. Himont and Mitsui have licensed Stauffer Chemical to make and sell the new catalyst in North and South America. Stauffer is a joint-venture partner with Hercules in Texas Alkyls, which makes aluminum alkyls.

A catalytic polymerization still in its infancy is the group-transfer process invented at Du Pont. The technique produces homopolymers and random and block copolymers of such α,β -unsaturated carbonyl monomers as methacrylates. Molecular weight ranges are narrow, and end groups can be chosen to fit the use. The catalyst described by Du Pont chemists is tris(dimethylamino)sulfonium bifluoride, which is available from Carbolabs, New Haven, Conn. It is uncertain what catalysts will be used in commercial resin production or what their economic value may be.

Group-transfer polymerization is initiated by a trimethylsilyl ketal such as dimethylketene methyl trimethylsilyl ketal. Polymerization occurs at room temperature. With addition of each α,β -unsaturated monomer molecule to the chain, the trimethylsilyl group transfers to the new carbonyl oxygen. That transfer creates a new trimethylsilyl ketal group on the growing end of the chain. Chain sequence is controlled by the composition of the monomer mixture or the order of monomer addition. The nature of the end groups depends on the compounds used as initiators and chain-terminators.

After polymerization, oxidation is the second largest market segment for chemical process catalysts, according to Frost & Sullivan research-

Process catalysts to top \$1 billion in 1990

	1985		1990	
	Volume (millions of lb)	Value (\$ millions)	Volume (millions of lb)	Value (\$ millions)
PETROLEUM REFINING	4670	\$545	5160	\$ 620
Catalytic cracking	370	250	405	275
Reforming	4.5	23	4.7	24
Hydrocracking	1.8	36	2.0	40
Hydrotreating	28	77	38	104
Alkylation	4265	160	4710	177
CHEMICAL PRODUCTION	190	410	230	500
Polymerization	50	175	60	220
Alkylation	90	50	110	60
Hydrogenation	9.6	35	11	40
Dehydrogenation	3.7	10	4.6	12
Oxidation, ammoxidation, and oxychlorination	11	85	14	105
Ammonia, hydrogen, and methanol production	26	55	31	60
TOTAL	4860	\$955	5390	\$1120

Note: Figures may not total exactly because of rounding. Source: Frost & Sullivan

ers. This segment includes ammoxidation catalysts for production of acrylonitrile from propylene, ammonia, and oxygen, and oxychlorination catalysts for conversion of ethylene to ethylene dichloride. Chemical plants used 11 million lb of oxidation catalysts in 1985, worth \$85 million. That amount will increase at more than 4% annually to 14 million lb in 1990, valued at \$105 million.

Favorable economics may shift production of methacrylonitrile in coming years to ammoxidation of a mixed butene stream, say analysts at Catalytica Associates, Mountain View, Calif., a catalyst development research firm. So concludes the company in a study of the impact of future catalyst developments on the chemical industry. The current process is reaction of acetone and hydrogen cyanide to the cyanohydrin, followed by dehydration. Such a shift would increase consumption of ammoxidation catalysts.

But a shift away from acetone and hydrogen cyanide may be averted by the pricing of those compounds, which are both by-products. Acetone is a by-product of phenol production, and hydrogen cyanide is a by-product of the acrylonitrile process.

Other major catalytic chemical processes are hydrogenation and dehydrogenation. Hydrogenation catalysts can be platinum or palladium on supports or a finely divided nick-

el called Raney nickel. Industrial hydrogenations include conversion of benzene to cyclohexane, phenol to cyclohexanone for caprolactam production, edible oils to shortenings, inedible oils to saturated fatty acids as rubber additives, and a mixture of 20% 2,6- and 80% 2,4-dinitrotoluene to toluenediamines as an intermediate in toluene diisocyanate production.

Dehydrogenation catalysts are generally aluminum, chromium, and/or ferric oxides. Commercial dehydrogenations include conversion of butane to butenes, butenes to butadiene, and ethylbenzene to styrene.

Frost & Sullivan analysts predict almost 7%-per-year increases in use of hydrogenation catalysts to 11 million lb worth \$40 million in 1990 from 9.6 million lb valued at \$35 million in 1985. The firm forecasts nearly 4% growth yearly for dehydrogenation catalysts to 1.2 million lb in 1990, worth \$4.6 million, from 1 million lb in 1985, valued at \$3.7 million.

Among refinery catalysts, fluid catalytic cracking (FCC) catalysts have the greatest volume and show the fastest growth, according to Frost & Sullivan. Consumption of FCC catalysts will increase at almost 5% per year to 405 million lb in 1990, valued at \$275 million, from 370 million lb in 1985, worth \$250 million.

One reason for such high vol-

Product Report

umes and growth is the crucial role of FCC in increasing the yield of gasoline. From 35 to 60% of crude oil may pass through the "cat cracker" during refining. FCC converts gas oils at process temperatures from 400 to 700 °F to lighter hydrocarbons. Atmospheric gas oil (AGO) is a distillate boiling from 530 to 650 °F. Vacuum gas oil, taken off at 0.15 atm after AGO passes over, has a theoretical atmospheric boiling range of 650 to 1050 °F. FCC also increases the content of branched-chain and aromatic hydrocarbons, which raise gasoline octane levels.

A second reason for high volumes and growth of FCC catalysts is that they must be replaced more often than those for other refining processes.

Such a large market segment has attracted recent competition. Until 1982, Davison sold about 50% of FCC catalysts used in the U.S., Engelhard 30%, and Filtrol 20%, say Frost & Sullivan researchers. In 1982,

Katalistiks opened a U.S. sales office, and in 1985, Akzo Chemie America's Ketjen Catalysts division started its 90 million lb-per-year plant in Pasadena, Tex. At present, Katalistiks sells an estimated 10% of U.S. FCC catalysts and Ketjen 5%, with Davison, Engelhard, and Harshaw/Filtrol having lost slightly in proportion. The result has been lower prices as catalyst producers have fought to win or keep market share.

Davison, for example, has restructured its business to reduce costs and has kept up its research and technical service programs, says James J. Blazek, technical vice president. One technical service effort is analysis of equilibrium catalysts for refiners, regardless of whether those refiners are Davison customers. The company's technicians now analyze 7000 samples of equilibrium catalyst daily for about two dozen such characteristics as activity, surface area, and metals content with a turnaround time of five days. Sam-

ples come from 97% of all refineries in the U.S. and Canada.

Equilibrium catalyst is the total catalyst that is actually in the fluid catalytic cracker at any one time. Refiners periodically add a portion of fresh catalyst to the cracker. Changes in feedstock or operating conditions also affect the total state of the catalyst, and analyses of equilibrium catalysts reflect trends or problems. For example, hydrothermal deactivation from the leakage of water or steam into the catalyst regenerator produces different changes in pore volume, average pore diameter, and apparent bulk density from purely thermal deactivation.

FCC catalysts are zeolites supported on aluminum silicates. The dozen or so types differ as to particle size and zeolite composition, which may range from all-natural to all-synthetic. In addition to marketing a broad line of these types, Davison also supplies catalysts

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treated with additives to tailor them to particular refinery needs. Product manager John Juracek Jr. calls additives the company's handle on supplying custom catalysts.

One such additive, a noble metal supported on alumina, promotes the combustion of carbon monoxide to carbon dioxide in the regenerator. Another, a metal salt, promotes oxidation of sulfur dioxide to the metal sulfate, which is reduced to hydrogen sulfide for removal on return of the catalyst to the cracker.

Although all such additives are vital to their functions, perhaps the most important just now are proprietary zeolites for octane enhancement. That's because the Environmental Protection Agency is following a schedule for gradually eliminating lead additives in gasoline. Refiners find that using so-called octane catalysts on the huge volumes of hydrocarbons that flow through their FCC units is more economical than adding catalytic

reforming capacity or blending oxygenated additives into the gasoline. Octane catalysts contribute two to three more octane numbers to gasoline in comparison with conventional FCC catalysts.

About two more octane numbers result from increasing the olefin content and one number from raised aromatics levels. The Davison octane additive lowers the yield of gasoline and produces more C₃ and C₄ hydrocarbons. Refiners can subject the C₃-C₄ stream to alkylation, however, to restore some gasoline yield.

Indeed, alkylation catalysts are the most valuable class of refinery catalysts after those for FCC. One example of alkylation is reaction of isobutane with propylene. Although hydrofluoric acid is more costly than sulfuric, it is coming into wider use to catalyze alkylations owing to the fewer environmental problems with its use.

Frost & Sullivan analysts note that

hydrofluoric acid was used in 40% of alkylation capacity in 1978 and in 46% by 1983. Slow, steady growth at 2% per year is forecast for those commodity acids to 4.71 billion lb worth \$177 million in 1990 from 4.27 billion lb valued at \$160 million in 1985. Many chemical companies supply sulfuric acid and hydrofluoric acid to refineries, and many refineries have their own sulfuric acid plants.

After FCC and alkylation, two other important refining processes are hydrotreating and hydrocracking. Hydrotreating is a mild hydrogenolysis of nitrogen, oxygen, and sulfur compounds and olefins to ammonia, water, hydrogen sulfide, and paraffins. The output stream from the hydrotreater goes to the cat cracker. Hydrocracking is catalytic cracking of refining residues to lighter, more highly branched hydrocarbons in the gasoline range in a hydrogen atmosphere. The output stream from hydrocracking is defi-

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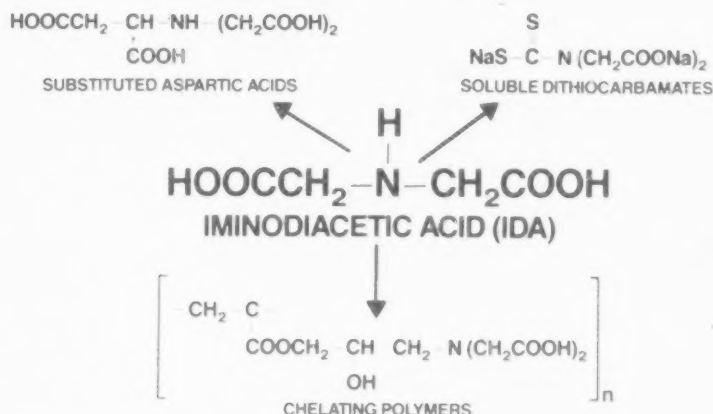


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Product Report

cient in octane-building olefins and aromatics and must usually be upgraded in octane by catalytic reforming. Hydrocracking of naphtha is also a source of petroleum gases.

Hydrotreating catalysts are cobalt or nickel molybdate or nickel tungstate on an alumina or zeolite support. The composition of metal salts varies according to whether the emphasis is on desulfurization or denitrification. Akzo Chemie America, American Cyanamid, Katalco, and Shell Chemical supply 90% of the U.S. market.

Hydrocracking catalysts include nickel, cobalt, molybdenum, tungsten, platinum, or palladium on aluminum silicate or zeolite supports. The leading suppliers to U.S. refineries are American Cyanamid, Shell Chemical, and UOP, a subsidiary of Allied-Signal, with some participation by Harshaw/Filtrol.

The level of activity of both hydrotreating and hydrocracking increases with refining of heavier, dirtier, more sour crudes. Though industry observers predict a bright long-term future for catalysts of these processes, the current ample supply of light, sweet crudes will restrict their growth for an indefinite time to come. Thus the FCC unit will keep its title as gasoline machine at U.S. refineries for now. Growth of hydrotreating catalysts also is restricted by activity to regenerate them in forms as active as fresh catalyst.

Frost & Sullivan studies indicate that hydrotreating catalyst use will rise at 6% yearly to 104 million lb worth \$38 million in 1990 from 77 million lb valued at \$28 million in 1985. Hydrocracking catalysts will grow at an average annual rate of about 2% to 40 million lb worth \$2 million in 1990 from 36 million lb valued at \$1.8 million in 1985.

A fifth major catalytic refinery process is catalytic reforming. That process dehydrogenates and isomerizes naphtha at 850 to 1000 °F to increase its content of branched-chain hydrocarbons and aromatics. Hydrogen from reforming goes to hydrotreating and hydrocracking. Reforming catalysts are platinum or platinum plus rhenium supported on alumina. American Cyanamid,

Continued on page 46



Harshaw/Filtrol researcher prepares to calcine catalyst in oven

Engelhard, and UOP have about 75% of the U.S. reforming catalyst market.

Levels of reforming activity at refineries vary directly with gasoline demand and inversely with the amounts of lead additives allowed in gasoline. Because they expect gasoline demand to decline over the next five years, Frost & Sullivan analysts predict only 0.5% annual growth in reforming catalyst consumption during the period. U.S. refineries used 4.5 million lb of such catalysts, worth \$23 million, in 1985. In 1990, they will use 4.7 million lb, valued at \$24 million.

Although not strictly a refining step, the Claus process to recover sulfur from hydrogen sulfide in refinery gases is an important one. This process oxidizes part of the hydrogen sulfide to sulfur dioxide, which is then combined with more hydrogen sulfide to produce sulfur. Alumina is the catalyst. Such firms as Harshaw/Filtrol supply the catalysts, and this company recently has developed a proprietary nonalumina catalyst that is said to function exceptionally well when carbon disulfide and carbonyl sulfide are present in the gases. Those compounds could be produced if hydrocarbons get into the reactor.

Although catalysts are already important in chemical and oil-refining processes, their roles are expected to expand vastly in coming years as

research uncovers new catalyst substances and catalytic processes. Harold Witcoff of Chem Systems, London, says the catalyst-producing industry has several objectives for the future, including the advance of catalysis theory to a priori catalyst design, improving selectivities in processes currently carried out, improving catalyst activity, deriving catalysts for new reactions, and devising stereoselective catalysts.

Witcoff has identified many promising areas of future research in a study on selected catalyst developments he did for Chem Systems, which is headquartered in Tarrytown, N.Y. These areas include phase-transfer catalysts, catalysts for asymmetric synthesis, multifunctional catalysts, intercalated catalysts, and zeolites.

Phase-transfer catalysts are usually quaternary ammonium salts, which are compatible with both water and organic solvents. The quaternary cations usher reactants and products back and forth between immiscible liquids. Phase-transfer catalysts mediate reactions of nonpolar with polar or ionic reactants. Without them, industrial chemists might have to use costly solvents, such as dimethylformamide, that are difficult to recover, or multiply the number of steps needed to make a product.

Witcoff points out that the most important current phase-transfer cat-

alytic process is production of polycarbonate resins from bisphenol A and phosgene. A quaternary ammonium salt brings phosgene out of methylene chloride into a sodium hydroxide solution of bisphenol A for reaction. The resin is extracted back into the methylene chloride. Thus phase-transfer catalysis mediates a reaction between a water-sensitive, nonpolar gas and an ionic salt. Before the invention of this process, resin makers converted phosgene to diphenyl carbonate, transesterified this with bisphenol A, and distilled the phenol for reuse.

A second current use is esterification of ampicillin into a prodrug. A prodrug is a compound that lasts longer in the body, because the prodrug must be converted to active compound to exert its effect. In addition, some prodrugs are better able to reach some sites of the body than the active drugs. In phase-transfer catalytic esterification of ampicillin, a quaternary ammonium salt brings an alkyl bromide out of chloroform into an aqueous solution of the potassium salt of ampicillin. The ester is extracted into the chloroform after reaction at room temperature. Alternative esterification reactions run the risk of hydrolyzing the β -lactam ring.

The most important catalytic process for asymmetric synthesis is that developed by Monsanto to hydrogenate an α -acetaminocinnamic acid to an L-hydrocinnamic acid, which is an intermediate for production of L-dihydroxyphenylalanine (L-dopa), a drug used to treat Parkinson's disease. The catalyst is a chelate of rhodium(I) with optically active bis(phenyl-2-methoxyphenylphosphino)ethane. Witcoff suggests that the process might be adapted to making L-phenylalanine, an intermediate in production of the sweetener aspartame.

Another catalytic asymmetric synthetic technique that might find wide commercial use is the asymmetric epoxidation of allylic alcohols. The method was invented by organic chemistry professor K. Barry Sharpless of Massachusetts Institute of Technology. In such reactions, titanium tetrakisopropoxide and diethyl D- or L-tartrate mediate epoxidation by *tert*-butyl hydropere-

oxide. Chemists can select the epoxide enantiomorph to be produced by choosing the appropriate tartrate isomer. Simply sketching out the structure of the allylic alcohol lets chemists predict which enantiomorph will result.

Candidates for catalytic asymmetric syntheses include drugs and insect pheromones. Often only one optical isomer of a drug is active and the other either inactive or harmful. For pheromones, making only the active enantiomorph produces a more potent compound for pest control.

A technique that achieves asymmetric synthesis by phase-transfer catalysis has been invented by process engineering chemists at Merck Sharp & Dohme. Their process alkylates 6,7-dichloro-5-methoxy-2-phenyl-1-indanone to the *S*-(+)-2-methyl compound with methyl chloride in 92% enantiomeric excesses and 95% yields. The optically active phase-transfer catalyst is *N*-*p*-trifluoromethylbenzylcinchoninium bromide, and the solvents are aqueous sodium hydroxide and chloroform-toluene. The product is an interme-

diate in production of *S*-(+)-indacinone.

S-(+)-Indacinone is a drug that eliminates uric acid through the urine to keep a proper balance of that compound in the body. The *R*-(-)-isomer increases urine production and sodium excretion. Disorders of uric acid metabolism include gallstones and gout. Increased urine production and sodium excretion aid in treating hypertension. Controlling the ratios of both enantiomorphs may produce the optimum level of each type of drug activity.

Among the multifunctional catalysts for which Witcoff sees much future promise, the most important in current use is one for catalytic reforming. A multifunctional catalyst has two different kinds of active sites that are close to one another. One kind of active site catalyzes a reaction of the product formed at the other. Continuous conversion of the intermediate product shifts the equilibrium to keep the overall reaction going.

The reforming catalyst has a noble metal supported on silica. Acidic sites on silica mediate such conversions as methylpentanes to cyclohexane. The noble metal dehydrogenates cyclohexane to benzene. The overall effect is to increase the amounts of aromatics formed.

Both the intercalated catalysts and zeolites whose potential Witcoff has studied are examples of shape-selective catalysts. The interstices of these minerals are of sizes and shapes that allow entry or exit of some molecules but not others. Intercalated catalysts, also called pillared clays, have large spaces between layers.

One such clay, smectite, was the original cracking catalyst at oil refineries in the 1930s. When zeolites with their smaller cavities were found superior, refiners abandoned smectite. The only commercial use of pillared clays today is conversion of oleic acid to dimer acid.

Nevertheless, Witcoff says that catalyst researchers are reinvestigating pillared clays, because the many useful processes that have been developed around zeolites suggest a bright future for shape-selective catalysts generally. One possibility he cites is polymerization. The cavities

between layers may produce uniform molecular weight distributions, and the cavities may be large enough to allow polymer molecules to exit after formation.

But pillared clays may be useful to catalyze reactions of any large molecules. Steroids and antibiotics are of such a molecular size that may fit into the interstices of pillared clays but not those of zeolites.

The biggest use for zeolites is in fluid cracking catalysts. Witcoff says that much work is under way to develop hydrocracking catalysts based on them also. Zeolites doped with metals might yield catalysts that are more active and less susceptible to poisoning, and that produce more-uniform products.

Another important use is production of ethylbenzene, where zeolites are replacing aluminum chloride. Zeolite catalysts are also used in the Mobil-Hoechst process to make *p*-methylstyrene. Those catalysts produce preferentially the *p*-ethyltoluene precursor from toluene and ethylene. Other alkylation processes for toluene give a mixture of ortho, meta, and para isomers. The end-product mixture, called vinyltoluene, is used as a crosslinking agent in unsaturated polyesters.

Plastics producers were interested in *p*-methylstyrene to replace styrene because of the high cost of benzene relative to toluene during the oil shortages of the past decade. The current plentiful supply of oil and low price of benzene have forced abandonment of *p*-methylstyrene. But a return of oil shortages could encourage producers to take up the process again.

Mobil Chemical has developed a zeolite-catalyzed process to convert methanol made from synthesis gas to gasoline. Another Mobil process not used now converts methanol to olefins, mostly propylene and butylenes, which can be polymerized to gasoline and middle distillates. UOP has developed a zeolite-catalyzed process to make methylated benzenes from ethane and propane. All of these technologies make gasoline and octane-raising components, and they could become useful with the recurrence of oil shortages. □



Worker tests catalyst at Engelhard's Menlo Park, N.J., research facility